grouping the molecules based on similarity of their respective descriptions and without consideration of their respective activity characteristics, so as to define groups of structurally similar molecules;

selecting at least one of the groups of structurally similar molecules based on an extent to which the molecules in the selected group have the given activity;

for each of the at least one selected group, identifying at least one molecular feature set common to all of the molecules in the selected group; and

outputting data indicative of at least one identified molecular feature set.

71. (Amended) The computerized method of claim 70, wherein the clustering algorithm comprises Self-Organizing-Map (SOM) clustering.

72. (Amended) The computerized method of claim 69, wherein selecting at least one of the groups based on an extent to which the molecules in the selected group have the given activity comprises:

selecting a group because the group contains at least a predetermined number of molecules that have the given activity.

73. (Amended) The computerized method of claim 69, wherein selecting at least one of the groups based on an extent to which the molecules in the selected group have the given activity comprises:

selecting a group because at least a predetermined percent of the molecules in the group have the given activity.

83. (Amended) [illegible]

defines, respectively for each molecule, a molecular structure and an activity [illegible]

operating the computer to establish for each molecule a respective description vector, by comparison of the molecule's molecular structure to a set of molecular substructure keys;

operating the computer to apply a clustering algorithm so as to sort the molecules into groups based on similarity of their respective description vectors and without consideration of their respective activity characteristics;

operating the computer to select at least one of the groups based on an extent to which the molecules in the selected group have the given activity;

operating the computer to identify, for each of the at least one selected group, a maximum common substructure of the molecules in the selected group; and

outputting from the computer data indicative of at least one identified molecular feature set.

84. (Amended) A computerized method of identifying a molecular feature set likely to be responsible for a given activity, based on a set of input data that represents molecules and that defines respectively for each molecule a molecular structure and an activity characteristic, the method comprising:

(a) establishing for each molecule a respective description, by comparison of the molecule's molecular structure to a set of molecular substructure keys;

(b) grouping the molecules based on similarity of their respective descriptions and without consideration of their respective activity characteristics, so as to define groups of structurally similar molecules;

(c) selecting at least one of the groups of structurally similar molecules based on an extent to which the molecules in the selected group have the given activity;

(d) for each of the at least one selected group, identifying at least one molecular feature set common to all of the molecules in selected group;

molecular substructure keys, and then repeating elements (a) through (d) using the modified set of molecular substructure keys as the set of molecular substructure keys; and

86. (Amended) The method of claim 84, wherein grouping the molecules based on similarity of their respective descriptions comprises Self-Organizing-Map (SOM) clustering the molecules based on their respective descriptions.

90. (Amended) A processing system for modeling chemical structure-activity relationships through artificial intelligence analysis of an input data set representing molecules, each of the molecules having a set of features and an activity characteristic, the processing system comprising, in combination:

means for establishing for each molecule a respective description, by comparison of the molecule's molecular structure to a set of molecular substructure keys;

means for grouping the molecules based on similarity of their respective descriptions and without consideration of their respective activity characteristics, so as to define groups of structurally similar molecules;

means for selecting at least one of the groups of structurally similar molecules based on an extent to which the molecules in the selected group have the given activity;

means for identifying at least one molecular feature set common to all of the molecules in each of at least one selected group; and

means for outputting data indicative of at least one identified molecular feature set.

Remarks

1. Response to Rejections under 35 U.S.C. § 112, First Paragraph

In the Office Action mailed July 16, 2001, the Examiner rejected all pending claims 69-

rejection, because the specification as filed does sufficiently teach each of the items noted by the